

=> b reg
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STRUCTURE FILE UPDATES: 16 AUG 2009 HIGHEST RN 1174375-84-8
 DICTIONARY FILE UPDATES: 16 AUG 2009 HIGHEST RN 1174375-84-8

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d que sta l8

L5 STR
 8 9
 G1 G1
 ||| |||
 Hy~C~Hy~Cb~N~C~Cb
 1 2 3 4 5 6 7

VAR G1=O/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E7 C E2 N AT 1

ECOUNT IS E4 C E1 O AT 3

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L6 225 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (NC5-NC2NC3 AND
 OC4)/ES

L8 14 SEA FILE=REGISTRY SUB=L6 SSS FUL L5

100.0% PROCESSED 159 ITERATIONS

14 ANSWERS

SEARCH TIME: 00.00.01

=> b zcap
 FILE 'ZCAPLUS' ENTERED AT 14:49:04 ON 17 AUG 2009
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 17 Aug 2009 VOL 151 ISS 8

FILE LAST UPDATED: 16 Aug 2009 (20090816/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate
substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family
of databases have been updated to include new citing references
information. This enhancement may impact record import into
database management software. For additional information, refer
to NEWS 9.

=> d bib abs hitstr 117 tot

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS ON STN (Continued)
 RN 2005:82712 ZCAPLUS
 DN 143:229891
 II Diazabicyclic aryl derivatives as nicotinic acetylcholine receptor ligands; their preparation and pharmaceutical compositions
 IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyhring; Ahning, Philip K.; Timmermann, Daniel B.
 PA Neurosearch A/S, Den.
 SO PCT Int. Appl. 49 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

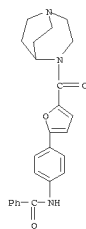
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EP-----1713810	A1	20061025	2005EP-000716606	20050201
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MX--2006008749	A	20061030	2006MX-000008749	20060802
IN--200602846	A	20070706	2006IN-000002846	20060803
PRAI 2004DK-00000169	A	20040204		
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2005WO-EP0050405	W	20050201		
OS CASREACT 143:229891; MARPAT 143:229891				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a group of diazabicyclic aryl derivs. I, including its enantiomers, N-oxides, prodrugs, and pharmaceutically acceptable salts, which are cholinergic ligands at the nicotinic acetylcholine receptors. In compds. I, n is 1-3; X and Y are independently selected from (un)substituted aromatic monocyclic/polycyclic carbocycles/heterocycles; Z is an (un)substituted monocyclic heterocycle, amino, (thio)carbonylamino, imidamido, ureido, thioureido, or guanidino; and L is a bond, CH₂, CH₂CH₂, CH=CH, C≡C, bond, O, S, SCH₂, etc. The invention also relates to the preparation of I, pharmaceutical compds. containing I or a pharmaceutically acceptable salt of I, together with at least one pharmaceutically acceptable carrier or diluent, as well as to the use of the compds. for the treatment of diseases and disorders associated with nicotinic acetylcholine receptors. 3-Quinuclidinone hydrochloride was condensed with hydroxylamine and ring expansion followed by reduction with LiAlH₄ resulted in the formation of 1,4-diazabicyclo[3.2.2]nonane (II). II was acylated with 5-(4-nitrophenyl)-2-furoyl chloride (preparation in situ from the corresponding acid is given) to give III. Palladium-catalyzed hydrogenation of III followed by addition to Et isocyanate gave diazabicyclic derivative IV. Compound IV expressed IC₅₀ value of 0.56 nM in a study on the

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS ON STN (Continued)
 RN 2005:82712 ZCAPLUS
 DN 143:229891
 II Diazabicyclic aryl derivatives as nicotinic acetylcholine receptor ligands; their preparation and pharmaceutical compositions
 IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyhring; Ahning, Philip K.; Timmermann, Daniel B.
 PA Neurosearch A/S, Den.
 SO PCT Int. Appl. 49 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

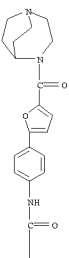
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EP-----1713810	A1	20061025	2005EP-000716606	20050201
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BR--2005006881	A	20070626	2005BR-000006881	20050201
JP--200750527	T	20070726	2006JP-000551845	20050201
US--20080227772	A1	20080918	2006US-000586749	20060721
MX--2006008749	A	20061030	2006MX-000008749	20060802
IN--200602846	A	20070706	2006IN-000002846	20060803
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2004DK-000000839	A	20040528		
2004US-00574946P	P	20040528		
2005WO-EP0050405	W	20050201		
OS CASREACT 143:229891; MARPAT 143:229891				
GI				



RN 862851-87-4 ZCAPLUS
 CN Benzamide, 4-amino-N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]- (CA INDEX NAME)

L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS ON STN (Continued)

PAGE 1-A

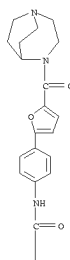


PAGE 2-A



RN 862851-89-6 ZCAPLUS
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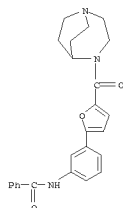
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L17 ANSWER 1 OF 2 ZCAPLUS COPYRIGHT 2009 ACS ON STN (Continued)
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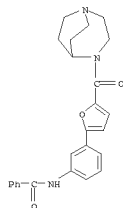
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 CN Benzamide, N-[3-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]- (CA INDEX NAME)



RN 862852-30-0 ZCAPLUS
 CN Benzamide, N-[3-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

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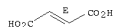
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CM 2

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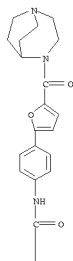
Double bond geometry as shown.



L17 ANSWER 1 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN (Continued)

RN 862852-33-3 SCAPLUS
 CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-2-nitro-, hydrochloride (1:1) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

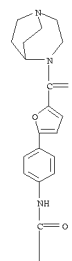


● HCl

RN 862852-43-5 SCAPLUS
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L17 ANSWER 1 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN (Continued)

PAGE 1-A



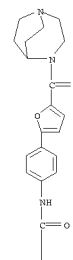
PAGE 2-A



II 862851-88-5P, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-4-nitrobenzamide 862851-90-9P, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-3-nitrobenzamide 862852-35-5P, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-4-nitrobenzamide hydrochloride 862852-37-7P, N-[4-[5-[(1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl]furan-2-yl]phenyl]-3-nitrobenzamide hydrochloride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of diazabicyclic aryl derivs. as nicotinic acetylcholine receptor ligands)
 RN 862851-88-5 SCAPLUS
 CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-4-nitro- (CA INDEX NAME)

L17 ANSWER 1 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN (Continued)

PAGE 1-A

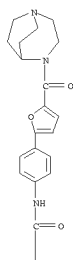


PAGE 2-A



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PAGE 1-A



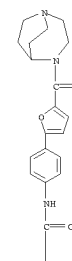
L17 ANSWER 1 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN (Continued)

PAGE 2-A



RN 862852-35-5 SCAPLUS
 CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-4-nitro-, hydrochloride (1:1) (CA INDEX NAME)

PAGE 1-A



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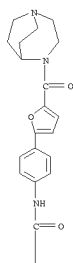


● HCl

RN 862852-37-7 SCAPLUS
 CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-3-nitro-, hydrochloride (1:1) (CA INDEX NAME)

L17 ANSWER 1 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN (Continued)

PAGE 1-A



PAGE 2-A



● HCl

OSC.G 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
 RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN

AN 2004:740327 SCAPLUS

DN 141:260783

TI Preparation of diazabicyclic aryl derivatives as cholinergic ligands at

the nicotinic acetylcholine receptors

IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen,

Tino Dyhring; Ahning, Philip K.

PA Neurosearch A/S, Den.

SO PCT Int. Appl., 40 pp.

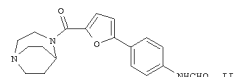
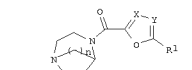
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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FW: BW, GH, GM, KE, LS, MW, ME, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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US--20060148789	A1	20060706	2005US-000547157	20050826
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HK-----1084110	A1	20070928	2006HK-000104352	20060411
PRAI 2003DK-000000310	A	20030227		
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2003DK-000000940	A	20030624		
2003US-00482022P	P	20030625		
2004WO-EP0050079	P	20040204		
OS MAPPAT 141:260783	W			
GI				



AB Title compds. represented by the formula I (wherein X, Y = independently CR2, CR3, N; R1 = H, (cyclo)alkyl, halo, etc.; R2, R3 = independently H, (cyclo)alkyl, alkyl, nitro, aryl, etc.; n = 1-3; and their enantiomers, any mixture of enantiomers, a prodrug, or pharmaceutically acceptable salts thereof) were prepared as cholinergic ligands at the nicotinic acetylcholine receptors. For example, reaction of (1,4-diazabicyclo[3.2.2]non-4-yl)-5-(4-aminophenyl)furan-2-ylmethanone and

L17 ANSWER 2 OF 2 SCAPLUS COPYRIGHT 2009 ACS on SIN (Continued)

Et formate gave II in 53% yield. II showed inhibition of 3H- α -Bungarotoxine binding with IC50 value of 0.017 μ M. Thus, I and their pharmaceutical compns. are useful as cholinergic ligands at the nicotinic acetylcholine receptors for the treatment of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances (no data).

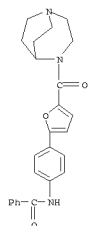
IT 753499-87-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diazabicyclic aryl derivs. as cholinergic ligands at the nicotinic acetylcholine receptors)

RN 753499-87-5 SCAPLUS

CN Benzamide, N-[4-{5-[(1,4-diazabicyclo[3.2.2]non-4-yl)carbonyl]-2-furanyl}phenyl]- (CA INDEX NAME)

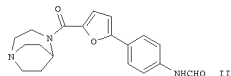
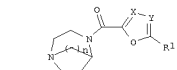


OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
 RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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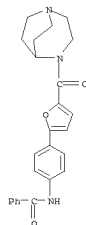
L18 ANSWER 1 OF 1 SCAPLUS COPYRIGHT 2009 ACS ON STM (Continued)
 AN 2004:740327 ZCAPLUS
 DN 141:260783
 TI Preparation of diazabicyclic aryl derivatives as cholinergic ligands at the nicotinic acetylcholine receptors
 IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyhring; Ahning, Philip K.
 PA Neurosearch A/S, Den.
 SO PCT Int. Appl., 48 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO--2004076453	A1	20040910	2004WO-EP0050079	20040204
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DE, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, ME, NA, NI, PW, BW, GH, GM, KE, LS, MM, ME, SD, SL, SZ, TE, UG, ZM, ZW, AT, BE, BG, CH, CI, CT, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, SR, TH, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	A1	20040910	2004AU-000215658	20040204
AU--2004215658	A1	20040910	2004CA-002518675	20040204
CA-----2518675	A1	20051130	2004EP-000707948	20040204
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BR--2004007216	A	20060222	2004CN-000002423	20040204
CN-----1738820	A	20070523	2006JP-000502001	20040204
CN-----1317280	C	20060824	2006JP-000502001	20040204
JP--2006019208	T	20080630	2005RU-00018997	20040204
NZ-----540998	A	20080630	2005US-000547157	20050826
RU-----2338746	C2	20081120	2005IN-000002058	20060411
US--20060148789	A1	20070831	2006HK-000104352	20060411
IN-----200502058	A	20070928	2003JUS-000000310	20030227
HK-----1084110	A	20030227	2003JUS-004498719	20030227
PRAI 2003JUS-000000310	A	20030625	2003JUS-000000940	20030625
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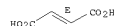
AB Title compds. represented by the formula I [wherein X, Y = independently CR2, CR3, N; R1 = H, (cyclo)alkyl, halo, etc.; R2, R3 = independently H, (cyclo)alkyl, alkyl, nitro, aryl, etc.; n = 1-3; and their enantiomers, any mixture of enantiomers, a prodrug, or pharmaceutically acceptable salts thereof] were prepared as cholinergic ligands at the nicotinic acetylcholine

L18 ANSWER 1 OF 1 SCAPLUS COPYRIGHT 2009 ACS ON STM (Continued)
 receptors. For example, reaction of (1,4-diazabicyclo[3.2.2]non-4-yl)-5-(4-aminophenyl)furan-2-ylmethanone and Et formate gave II in 53% yield. II showed inhibition of 3H- α -Bungarotoxin binding with IC50 value of 0.017 μ M. Thus, I and their pharmaceutical compns. are useful as cholinergic ligands at the nicotinic acetylcholine receptors for the treatment of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances (no data).
 IT 753499-88-6P 753499-91-1P 753499-92-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of diazabicyclic aryl derivs. as cholinergic ligands at the nicotinic acetylcholine receptors)
 RN 753499-88-6 ZCAPLUS
 CN Benzanide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)
 CM 1
 CRN 753499-87-5
 CMF C25 H25 N3 O3



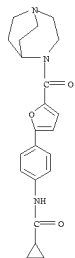
CM 2
 CRN 110-17-8
 CMF C4 H4 O4

Double bond geometry as shown.

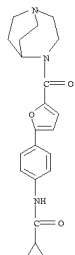


RN 753499-91-1 ZCAPLUS
 CN Cyclopropanecarboxamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

L18 ANSWER 1 OF 1 SCAPLUS COPYRIGHT 2009 ACS ON STM (Continued)

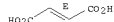


RN 753499-92-2 ZCAPLUS
 CN Cyclopropanecarboxamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)
 CM 1
 CRN 753499-91-1
 CMF C22 H25 N3 O3



CM 2
 CRN 110-17-8
 CMF C4 H4 O4

Double bond geometry as shown.



OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L18 ANSWER 1 OF 1 SCAPLUS COPYRIGHT 2009 ACS ON STM (Continued)
 RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 14:29:56 ON 17 AUG 2009)

FILE 'ZCAPLUS' ENTERED AT 14:30:10 ON 17 AUG 2009

L1 1 US20080227772/PN

FILE 'REGISTRY' ENTERED AT 14:30:24 ON 17 AUG 2009

FILE 'ZCAPLUS' ENTERED AT 14:30:24 ON 17 AUG 2009

L2 TRA L1 1- RN : 74 TERMS

FILE 'REGISTRY' ENTERED AT 14:30:24 ON 17 AUG 2009

L3 74 SEA L2

L4 46 L3 AND NC5-NC2NC3/ES AND OC4/ES

L5 STR

L6 225 (NC5-NC2NC3 AND OC4)/ES

L7 2 L5 SAM SUB=L6

L8 14 L5 FULL SUB=L6

SAV TEM J749C1G2/A L8

L9 11 L8 AND L3

L10 3 L8 NOT L9

L11 2599 C25H25N3O3

L12 4 L11 AND L6

L13 3 L12 AND L3

L14 1 L12 NOT L13

L15 11 L9,L13

L16 3 L10,L14

FILE 'ZCAPLUS' ENTERED AT 14:47:41 ON 17 AUG 2009

L17 2 L15

L18 1 L16

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